

A unified framework for the computation of polynomial quadrature weights and errors*

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Abstract

For the class of polynomial quadrature rules we show that conveniently chosen bases allow to compute both the weights and the theoretical error expression of a n -point rule via the undetermined coefficients method. As an illustration, the framework is applied to some classical rules such as Newton-Cotes, Adams-Bashforth, Adams-Moulton and Gaussian rules.

Key-words: Quadrature, undetermined coefficients method, degree of precision, orthogonal polynomial.

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1 Introduction

Most numerical integration schemes widely used in the applications are based on the class of polynomial quadrature. Here we present an unified framework for the simultaneous computation of weights and theoretical error of a n -point polynomial quadrature rule $Q_n(f)$. We aim to bring together the computation of the pair (weights, error) = (W_n, E_n) under a simple and unified framework. Our approach shows that it is possible to choose a particular polynomial basis relative to which the weights W_n are the solution of an upper triangular linear system, enabling so their recursive computation. At the same time, by extending conveniently the referred basis, we

*Dedicated to the memory of Bernard Germain-Bonne (1940–2012).

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obtain a (computable) criterium for the degree of precision of the rule and consequently the respective error expression E_n .

The upper triangular system, whose solution is the vector W_n of weights, is obtained by the technique known in numerical analysis as undetermined coefficient method (not to be confused with the same named method for ODE's). The undetermined coefficients method (UCM) is often employed for weights's computation, however this method has been set aside for the determination of E_n (see for instance the remarks in Gautschi [7], p. 176, and Evans [5], p. 69). To the best of our knowledge, our scheme for the simultaneous computation of the weights and error via the UCM is new.

In numerical quadrature one aims to approximate an integral $I(f) = \int_a^b f(x)dx$ by a n -point rule $Q_n(f) = \sum_{k=1}^n a_k f(x_k)$, and to obtain an expression or a bound for the error $E_n(f) = I(f) - Q_n(f)$. The coefficients a_i in $Q_n(f)$ are called the (quadrature) weights and the points x_i in a given set $\{x_1, \dots, x_n\}$ are usually called nodes (a.k.a. quadrature points, or abscissae). The rule $Q_n(f)$ is said to be polynomial interpolatory when it is exact for polynomials of degree less or equal to $n - 1$. That is, when $Q_n(p) = I(p)$ for all polynomials p of degree less or equal to $n - 1$. Hereafter when we refer to a rule we mean a polynomial quadrature rule.

Quadrature has a long history and is a classical subject, although it is still nowadays an active area of research (general references are, for instance, Atkinson [1], Davis and Rabinowitz [4], Gautschi [7] and Krylov [10]). There are *a priori* two main goals when dealing with numerical quadrature: the determination of the weights and respective theoretical error expression. Traditionally, in order to obtain the weights, one first determines the interpolating polynomial for a given panel $\{(x_1, f(x_1)), (x_2, f(x_2)) \dots, (x_n, f(x_n))\}$ and afterwards this polynomial is integrated. The interpolating polynomial is unique (and so are the weights of the rule) but it may be written in several different forms named after Lagrange, Newton, Hermite, Chebyshev, etc. Of course, this means that we can always write the interpolating polynomial in distinct polynomial bases.

In the classical literature the theoretical quadrature error is usually deduced from a particular expression representing the interpolation error – see Steffenson [14] for a survey on interpolation theory, and Berezin and Zhidkov [2], Ch. 2, for its applications. Consequently, the quadrature error deduction is based upon a panoply of analytical tools such as mean value theorems, integration by parts, Peano kernels, Euler-MacLaurin formula and so on. The usual approach for the computation of the pair (W_n, E_n) , where $W_n = (a_1, \dots, a_n)$, is done on a rule by rule basis leading usually to lengthy

and cumbersome calculations even for a small number n of nodes.

At the heart of our approach are conveniently chosen bases of polynomials relative to which we apply the undetermined coefficients method in order to compute the pair (W_n, E_n) . Only elementary results from linear algebra and numerical analysis are needed.

The paper is organized as follows. There are two sections, in the first one we prove the main result (Theorem 2.1), which points out an algorithm for computing the pair (W_n, E_n) . In the following section we illustrate its applicability to well known quadrature rules named after their creators: Newton-Cotes, Adams-Basforth, Adams-Moulton, and Gaussian rules. This shows the wide applicability of the algorithm previously referred. In particular, when applying Theorem 2.1 to Gaussian quadratures we recover (in Proposition 3.1) a well known closed form for their error expression.

We barely address here numerical computational issues since they are out of the scope of this work, and will be treated elsewhere. However, several symbolic/numerical tests were carried out in order to compute pairs (W_n, E_n) for the illustrative quadrature rules mentioned above. For, we developed a *Mathematica* code translating the algorithm in Theorem 2.1 and we have tested it on all the rules described in Section 3. The respective computed weights and error expressions were compared with those in tables spread in the literature. In particular, for a number of nodes $2 \leq n \leq 256$, the algorithm has been used to compute 100-digits precision pairs (W_n, E_n) for the ubiquitous and indispensable Gauss-Legendre rule.

2 Weights and error for a polynomial rule

In order to approximate the integral $I(f) = \int_a^b f(x)dx$, where f is assumed to be an integrable function in (a, b) , and of class $C^k([a, b])$ (where the integer k will be taken appropriately to each case), one constructs the rule

$$Q_n(f) = a_1 f(x_1) + a_2 f(x_2) + \cdots + a_n f(x_n), \quad (1)$$

from a given set $\{x_1, x_2, \dots, x_n\}$, with $n \geq 1$.

The rule $Q_n(f)$ is said to have degree of precision d , if $I(p) = Q_n(p)$ for all polynomials p of degree $\leq d$, and $I(p) \neq Q_n(p)$ for some polynomial p of degree $d + 1$. If $d = \deg(Q_n(f))$ denotes the degree of precision of the rule $Q_n(f)$, and f is of class C^{d+1} in $[a, b]$, the quadrature error is given by

$$E_n(f) = I(f) - Q_n(f) = \frac{I(p_{d+1}) - Q_n(p_{d+1})}{(d+1)!} f^{(d+1)}(\xi), \quad (2)$$

where ξ and p_{d+1} are respectively a certain point in (a, b) and a polynomial of degree $d + 1$ (cf. Gautschi [7], p. 178). We remark that the degree of precision of a rule cannot be greater than $(2n - 1)$ since, if p is a polynomial of degree n then $I(p^2)$ is positive.

In numerical analysis the undetermined coefficients method consists in solving the linear system arising from the equalities $Q_n(g_i) = I(g_i)$, for $0 \leq i \leq (n - 1)$, where g_i are the elements of a prescribed set of functions. In the context of polynomial quadrature this set will be a set of polynomials. The next theorem shows that when the UCM is applied to a conveniently chosen basis of polynomials, the weights are obtained recursively and, at the same time, the degree of precision d of the corresponding quadrature rule is easily found.

We denote by \mathbb{P}_s the linear space of real polynomials of degree less or equal to s . Suppose that x_1, x_2, \dots, x_n are $n \geq 1$ distinct real points and consider the basis $B_0 = \{\varphi_0(x), \varphi_1(x), \dots, \varphi_{n-1}(x)\}$ of \mathbb{P}_{n-1} , given by

$$\begin{cases} \varphi_0(x) = 1 \\ \varphi_j(x) = \varphi_{j-1}(x)(x - x_j), \quad 1 \leq j \leq n - 1. \end{cases} \quad (3)$$

The basis B_0 is known in some literature as Newton's basis (see Stiefenssen [14], p. 23). We complete the basis B_0 with other polynomials $q_n(x), q_{n+1}(x), \dots, q_{n+k}(x)$ to form a basis \mathbb{P}_{n+k} . Notably,

$$\begin{cases} q_n(x) = \varphi_{n-1}(x)(x - x_n) \\ q_j(x) = q_{j-1}(x)(x - x_r), \quad j \geq n + 1 \quad \text{with} \quad r \equiv j \pmod{n}, \end{cases} \quad (4)$$

where k is a nonnegative integer which will be later specified in accordance with the particular quadrature rule under consideration. Note that the points x_i ($1 \leq i \leq n - 1$) are roots for all the polynomials q_j defined in (4).

Theorem 2.1. *Let x_1, \dots, x_n be $n \geq 1$ distinct real quadrature points, $B_0 = \{\varphi_0(x), \dots, \varphi_{n-1}(x)\}$ the basis of \mathbb{P}_{n-1} defined in (3), and $B = B_0 \cup \{q_n(x), \dots, q_{n+k}(x)\}$ the basis of \mathbb{P}_{n+k} , defined in (4).*

- (a) *The undetermined coefficient method applied to the basis B_0 determines (uniquely) the weights a_i of the rule (1) for approximating the integral $I(f) = \int_a^b f(x)dx$. These weights are*

$$\begin{cases} a_n = \frac{I(\varphi_{n-1})}{\varphi_{n-1}(x_n)}, \\ a_i = \frac{I(\varphi_{i-1}) - \sum_{k=i+1}^n \varphi_{i-1}(x_k)a_k}{\varphi_{i-1}(x_i)}, \quad i = n - 1, n - 2, \dots, 1. \end{cases} \quad (5)$$

(b) The undetermined coefficient method applied to the basis B , determines the degree of precision $d = \deg(Q_n(f))$ as being the integer $d \geq n - 1$ for which

$$I(q_{d+1}) \neq 0 \quad \text{and} \quad I(q_j) = 0, \text{ for all } n \leq j \leq d. \quad (6)$$

(c) If f is of class $C^{d+1}([a, b])$, the error expression is

$$E_{Q_n}(f) = c_n f^{(d+1)}(\xi), \quad \text{with } c_n = \frac{I(q_{d+1})}{(d+1)!}, \quad (7)$$

for some $\xi \in (a, b)$.

Proof. (a) As the rule $Q_n(f)$ is polynomial, applying the UCM to the basis B_0 of the polynomials φ_i of degree $i \leq (n - 1)$, we have

$$Q_n(\varphi_i) = I(\varphi_i), \quad \text{for all } 0 \leq i \leq (n - 1). \quad (8)$$

The conditions (8) are equivalent to the linear system $Ax = b$ in the unknowns a_1, \dots, a_n , where $b = (I(\varphi_0), I(\varphi_1), \dots, I(\varphi_{n-1}))^T$. The matrix A is a $n \times n$ upper triangular matrix whose diagonal entries are $1, \varphi_1(x_2), \dots, \varphi_{n-1}(x_n)$. Furthermore, A is obviously nonsingular since x_{i+1} is not a root of φ_i , for $1 \leq i \leq n - 1$, and so $\det(A) \neq 0$. The (unique) solution of $Ax = b$ is obtained by backward substitution and is given by (5).

(b) Applying the UCM to the basis B , we get an overdetermined linear system $\tilde{A}x = \tilde{b}$, where x is the vector whose components are the weights, and the $(n + k) \times n$ matrix \tilde{A} and the vector \tilde{b} are, respectively, of the form

$$\tilde{A} = \begin{bmatrix} A \\ O \end{bmatrix}_{(n+k) \times n} \quad \tilde{b} = (I(\varphi_0), \dots, I(\varphi_{n-1}), I(q_n), \dots, I(q_{n+k}))^T, \quad (9)$$

where O denotes the zero matrix. The conditions (6) in the statement are equivalent to say that $d = \deg(Q_n(f))$ is the greatest integer $n + k$ for which the system $\tilde{A}x = \tilde{b}$ is compatible.

Let us now show that the degree d of the rule $Q_n(f)$ is given by the conditions (6). Consider p to be a polynomial of degree $n + k$ for some nonnegative integer k and write p as (unique) linear combination of the elements of the basis B of \mathbb{P}_{n+k} . That is,

$$p = \sum_{j=0}^{n-1} \alpha_j \varphi_j + \sum_{j=n}^{n+k} \alpha_j q_j.$$

Then,

$$Q_n(p) = \sum_{j=0}^{n-1} \alpha_j Q_n(\varphi_j) + \sum_{j=n}^{n+k} \alpha_j Q_n(q_j) = \sum_{j=0}^{n-1} \alpha_j Q_n(\varphi_j), \quad (10)$$

where the last equality follows from the fact that all points x_i are roots of the polynomials q_j . Furthermore, by linearity of the operator I , we have

$$I(p) = \sum_{j=0}^{n-1} \alpha_j I(\varphi_j) + \sum_{j=n}^{n+k} \alpha_j I(q_j). \quad (11)$$

As by (8), $Q_n(\varphi_j) = I(\varphi_j)$, we conclude from (10) and (11) that

$$I(p) - Q_n(p) = \sum_{j=n}^{n+k} \alpha_j I(q_j). \quad (12)$$

Therefore the degree of precision d cannot be less than $(n-1)$. As there exists a polynomial p_s of degree $s \leq 2n$ such that $I(p_s) \neq 0$, this implies that $I(q_s) \neq 0$ for an integer s such that $n \leq s \leq 2n$. It also follows easily from (12) that $Q_n(p) = I(p)$, for all polynomials p of degree $\leq d$, if and only if $I(q_j) = 0$ for all $n \leq j \leq d$. So, the conditions (6) hold.

(c) As all the quadrature points are roots of the polynomial q_{d+1} , we have $Q_n(q_{d+1}) = 0$. Then, it follows from (2) that the error's expression is given by (7). □

Remarks 2.1. 1) It becomes clear from the proof of Theorem 2.1 the reason why the UCM has been set aside for the computation of the degree of a rule. Indeed, if one had applied the UCM to another basis B , for instance the canonical basis of polynomials, the matrix \tilde{A} in (9) would not have the zero block (or equivalently the second term of the sum in (10) does not vanishes), and so it will be impossible to obtain the criterium (6) for the degree.

2) Implicit in the proof of the above theorem is the following algorithm. Given the nodes x_1, \dots, x_n and the bases B_0 and B ; (i) Compute the weights W_n using the recursion relation (5); (ii) Find the first indice $j \geq n$ such that $I(q_j) \neq 0$; (iii) $d = j - 1$ is the degree of the rule; (iv) Compute the coefficient c_n in (7); (v) Output W_n and E_n .

- 3) As the degree of precision of a rule cannot be greater than $2n$, it is only necessary to extend the basis B_0 to a basis B of \mathbb{P}_{2n} . It also follows from the proof of Theorem 2.1 that the polynomials q_j only need to satisfy the requirement of having all quadrature points as roots.
- 4) From Theorem 2.1, we can conclude that the quadrature weights a_i of a polynomial rule do not depend whether the quadrature points belong or not to the integration interval $[a, b]$. However, the value of the integrals $I(q_j)$ do depend on the points's location relative to the interval of integration. In the next section we show how the position of the quadrature points may influence the degree of the precision of a rule, for instance in the cases of the Newton-Cotes and Adams-Bashforth-Moulton rules.
- 5) The upper triangular system leading to the computation of the weight's vector W_n , has determinant equal to $\det(A) = \prod_{j=1}^{n-1} \varphi_j(x_{j+1})$. For n large and certain sets of nodes we can have $\det(A) \approx 0$. In this case we are facing an ill-conditioned problem which raises challenging computational issues.
- 6) It would be interesting to apply Theorem 2.1 to polynomial rules other than those treated in Section 3, such as the Clenshaw-Curtis, Patterson, Gauss-Konrad, etc. (see Evans [5] for a survey of other available rules, and references therein).

3 Applications to some classical integration rules

In this section we apply Theorem 2.1 to some classical rules in order to obtain their weights and the respective error's expression. To illustrate the wide applicability of our result we begin with rules with equally spaced nodes (Newton-Cotes and Adams-Bashforth-Moulton) followed by rules with unequally spaced points (Gaussian).

3.1 Weights and error for Newton-Cotes and Adams-Bashforth-Moulton rules

The abscissae for both Newton-Cotes (open or closed) rules and Adams-Bashforth-Moulton are equally spaced. In the rules of the first type all the quadrature points belong to the integration interval $[a, b]$ whilst for the second type there are points outside $[a, b]$. These particularities of the nodes have a decisive influence on the rule's degree. The next Lemma shows how

the abscissae's distribution relative to the integration interval will affect the values of the integrals $I(q_j)$ in Theorem 2.1. Although the results in Lemma 3.1 are scattered in the literature under somehow different formulations, we include a proof for the sake of completeness.

Lemma 3.1. *Let y_1, y_2, \dots, y_n be real points such that $y_i = y_{i-1} + h$, for some positive constant h , and $q_n(x) = (x - y_1)(x - y_2) \cdots (x - y_n)$.*

i) *If $y_1 = a$ and $y_n = b$, then*

$$\int_a^b q_n(x) dx = \begin{cases} 0 & \text{if } n \text{ is odd} \\ \neq 0 & \text{if } n \text{ is even.} \end{cases}$$

ii) *If $q_{n+1}(x) = q_n(x)(x - \tilde{y})$, with $\tilde{y} = y_1$ or $\tilde{y} \notin [y_1, y_n]$, then $\int_{y_1}^{y_n} q_{n+1}(x) dx \neq 0$.*

iii) *If $y_{n-1} = a$ and $y_n = b$, then $\int_a^b q_n(x) dx \neq 0$.*

Proof. The change of variables $\gamma : x \mapsto t$, defined by $x = y_1 + h \left(t + \frac{n-1}{2}\right)$, maps $y_1 \mapsto -\frac{n-1}{2}$, $y_2 \mapsto -\frac{n-1}{2} + 1, \dots, y_{n-1} \mapsto \frac{n-1}{2} - 1$, $y_n \mapsto \frac{n-1}{2}$, and $[a, b] \mapsto [-(n-1)/2, (n-1)/2]$.

If n is odd, the integral $\int_a^b q_n(x) dx$ is equal to the integral of an odd function and so it is zero. That is,

$$\int_a^b q_n(x) dx = h^{n+1} \int_{-\frac{n-1}{2}}^{\frac{n-1}{2}} t(t^2 - 1)(t^2 - 2^2) \cdots \left(t^2 - \frac{(n-1)^2}{4}\right) dt = 0.$$

If n is even, then $\int_a^b q_n(x) dx$ is equal to the integral of an even function:

$$\int_a^b q_n(x) dx = h^{n+1} \int_{-\frac{n-1}{2}}^{\frac{n-1}{2}} (t^2 - 1/4)(t^2 - 9/4) \cdots \left(t^2 - \frac{(n-1)^2}{4}\right) dt \neq 0.$$

For ii), we can write \tilde{y} as $\tilde{y} = y_1 + h \left(\frac{n-1}{2}\right) + r$, where r is some nonzero constant. Thus, $(x - \tilde{y}) = (x - (y_1 + h \left(\frac{n-1}{2}\right))) + r$, and so

$$\begin{aligned} \int_{y_1}^{y_n} q_{n+1}(x) dx &= \int_{y_1}^{y_n} q_n(x) \left[x - \left(y_1 + h \left(\frac{n-1}{2} \right) \right) \right] dx - r \int_{y_1}^{y_n} q_n(x) dx \\ &= K_1 - r K_2. \end{aligned}$$

Applying (i) and the same change of variables as before, it is easy to conclude: (a) When n is odd, then $K_2 = 0$ and K_1 is the integral of an

even function in $[-(n-1)/2, (n-1)/2]$, and so $\int_{y_1}^{y_n} q_{n+1}(x)dx \neq 0$; (b) when n is even, then $K_2 \neq 0$ and K_1 is the integral of an odd function in $[-(n-1)/2, (n-1)/2]$, thus $\int_{y_1}^{y_n} q_{n+1}(x)dx \neq 0$.

(iii): When x belongs to the open interval (y_{n-1}, y_n) the product $(x - y_1)(x - y_2) \cdots (x - y_{n-1})$ is positive and $(x - y_n)$ does not vanishes. Therefore, the integrand function $q_n(x)$ does not change sign in $[y_{n-1}, y_n]$, hence $\int_{y_{n-1}}^{y_n} q_n(x) \neq 0$. \square

Closed Newton-Cotes rules

In order to approximate $I(f) = \int_a^b f(x)dx$, the interval $[a, b]$ is divided into $(n-1)$ parts of equal length $h = \frac{b-a}{n-1}$, and the nodes are: $x_i = a + ih$, for $i = 0, 1, \dots, (n-1)h$. By a change of variables, one can consider the n nodes to be $t_1 = 0, t_2 = 1, \dots, t_n = n-1$. The integral $I(f)$ is

$$I(f) = \int_a^b f(x)dx = h \int_0^{n-1} g(t)dt,$$

with $g(t) = f(a + th)$. The rule $Q_n(f)$ is related to the rule

$$Q_n(g) = b_1g(0) + b_2g(1) + \cdots + b_ng(n-1)$$

by $Q_n(f) = hQ_n(g)$. The elements of the basis B_0 in (3) are $\varphi_0(t) = 1$, $\varphi_j(t) = \varphi_{j-1}(t)(t - (j-1))$, for $j = 1, 2, \dots, n-1$. The polynomials q_n and q_{n+1} in (4) are

$$q_n(t) = t(t-1) \cdots (t-(n-1)), \quad q_{n+1}(t) = t^2(t-1) \cdots (t-(n-1)).$$

By (5) of Theorem 2.1, the weights b_i for $Q_n(g)$ are given recursively by

$$\begin{cases} b_n = \frac{I(\varphi_{n-1})}{\varphi_{n-1}(n-1)} = \frac{\int_0^{n-1} \varphi_{n-1}(t)dt}{(n-1)!}, \\ b_i = \frac{I(\varphi_{i-1}) - \sum_{k=i+1}^n \varphi_{i-1}(k-1)b_k}{(i-1)!}, \end{cases}$$

where we have applied the fact that $\varphi_k(k) = k!$. The weights for the rule $Q_n(f)$ are $a_i = hb_i$. The degree of $Q_n(g)$ is at least $(n-1)$, and from Lemma 3.1-(i) the integral $I(q_n(t)) = \int_0^{n-1} t(t-1) \cdots (t-(n-1))dt$ vanishes when n is odd and is nonzero when n is even. Also, by (ii) of the same Lemma,

$I(q_{n+1}(t)) \neq 0$. Then, by Theorem 2.1, the degree d and the error expression $E_n(f)$ for a n -point Newton-Cotes rule are respectively,

$$\begin{cases} d = n - 1, & \text{if } n \text{ is even} \\ d = n, & \text{if } n \text{ is odd} \end{cases}$$

and

$$\begin{aligned} E_n(f) &= I(f) - Q_n(f) = h(I(g) - Q_n(g)) \\ &= h \frac{I(q_{d+1})}{(d+1)!} g^{(d+1)}(\tilde{\xi}) = h^{d+2} \frac{I(q_{d+1})}{(d+1)!} f^{(d+1)}(\xi), \end{aligned}$$

where the last equality follows from the fact that $g^{(k)}(t) = h^k f^{(k)}(a + th)$, and we are assuming that $f \in C^{d+1}([a, b])$. That is,

$$E_n(f) = h^{d+2} c_n f^{(d+1)}(\xi), \quad \text{with } c_n = \frac{I(q_{d+1})}{(d+1)!}. \quad (13)$$

Using an analogous procedure, it is now a simple exercise to obtain the pair (W_n, E_n) for a n -point open Newton-Cotes rule.

The Adams-Bashforth-Moulton rules

The Adams-Bashforth (AB) rules are the core of explicit methods for ODEs and the Adams-Moulton (AM) rules play a central role as implicit methods for ODEs with the same name (Henrici [9], Gautschi [7], Cheney [3]).

The (equally spaced) nodes for the AB rule are less or equal to a (where $[a, b]$ is the integration interval), while in the AM case the points a and b are quadrature points and there are no other abscissae in the interior of $[a, b]$. The Lemma 3.1 and Theorem 2.1 imply that both the AB and AM rules have degree of precision $d = (n - 1)$.

We now describe in detail the polynomial bases to be used and we determine the theoretical error expression for both rules.

The Adams-Bashforth rule

Given a constant step h and a fixed real number τ , consider $n \geq 2$ nodes $x_1 = \tau$, $x_2 = \tau - h$, \dots , $x_n = (\tau - (n - 1)h)$. The Adams-Bashforth rule aims to approximate the integral $I(f) = \int_{\tau}^{\tau+h} f(x)dx$ by

$$Q_n(f) = a_1 f(x_1) + \dots + a_n f(x_n).$$

Making the change of variables defined by $x = \tau + ht$, we have

$$I(f) = \int_{\tau}^{\tau+h} f(x)dx = h \int_0^1 f(\tau + ht)dt = h \int_0^1 g(t)dt.$$

The nodes x_i are mapped into $t_1 = 0, t_2 = -1, \dots, t_n = -(n-1)$. The quadrature rule for f is related to the rule for g by $Q_n(f) = h Q_n(g)$, with

$$Q_n(g) = b_1 g(0) + b_2 g(-1) + \dots + b_n g(1-n) = \sum_{k=1}^n b_k g(1-k). \quad (14)$$

As the integral $I(q_n) = \int_0^1 q_n(t)dt$, where $q_n(t) = \varphi_{n-1}(t)(t + (n-1))$, is obviously positive, then the degree of $Q_n(g)$ (and so the degree of $Q_n(f)$) is $d = n-1$. Therefore, the error of $Q_n(g)$ is $E_n(g) = h \frac{I(q_n(t))}{n!} g^{(n)}(\tilde{\xi})$ and so

$$E_n(f) = h^{n+1} c_n f^{(n)}(\xi), \quad \text{with } c_n = \frac{I(q_n(t))}{n!}, \quad \xi \in (a, b), \quad (15)$$

assuming f to be of class $C^n([a, b])$.

The Adams-Moulton rules

Likewise, we intend to approximate $I(f) = \int_{\tau}^{\tau+h} f(x)dx$ by the rule $Q_n(f) = \sum_{i=1}^n a_i f(x_i)$, but now the nodes are $x_1 = \tau + h, x_2 = \tau, x_3 = \tau - h, x_4 = \tau - 2h, \dots, x_n = \tau - (n-2)h$. Performing the same change of variables as in the previous rule, we transform the interval $[\tau - (n-2)h, \tau + h]$ into the interval $[0, 1]$, and the nodes x_i into the nodes $t_1 = 1, t_2 = 0, \dots, t_n = 2-n$. As before $Q_n(f) = h Q_n(g)$. Here the polynomial $q_n(t)$ is $q_n(t) = \varphi_n(t)(t - (2-n))$ and so, by Lemma 3.1-(iii), we obtain $I(q_n(t)) = \int_0^1 q_n(t)dt \neq 0$. Therefore $\deg(Q_n(f)) = (n-1)$ and from Theorem 2.1 it follows an expression for $E_n(f)$ similar to (15).

Remark 3.1. In the Adams-Bashforth-Moulton rules the nodes t_i are integers and so the application of the UCM leads to a linear system $Ax = b$, where A is a matrix of integer entries. The integrals $I(\varphi(t))$ are rational numbers. Therefore both the weights of W_n and the respective error coefficient c_n in (15) can be computed exactly if one uses a computer algebra system able to represent exactly rational numbers. Of course the same is true for the Newton-Cotes rules discussed previously.

3.2 Gaussian quadrature rules

Gaussian rules, first introduced by Gauss in [6], rely on the properties of orthogonal sets of polynomials (see Gautschi [8] for a recent account on the subject). A Gaussian rule $G_n(f) = \sum_{k=1}^n a_k f(x_k)$ is used to approximate the integral $I(f) = \int_a^b w(x)f(x)dx$, where the so-called weight function w is assumed to be a positive function defined in $[a, b]$, continuous, and integrable in (a, b) .

In the context of Gaussian quadratures the following L^2 inner product plays a central role

$$\langle g, h \rangle = \int_a^b w(x)g(x)h(x)dx. \quad (16)$$

The existence of an orthogonal polynomial basis $\{O_0, O_1, \dots, O_n\}$ for \mathbb{P}_n is guaranteed by the Gram-Schmit process, and it is common to call the elements of such bases by orthogonal polynomials. The most widely used sets of orthogonal polynomials are known by the names of Hermite, Laguerre, Jacobi, Chebyshev and Legendre polynomials. Lists of orthogonal polynomials, respective weight functions and integration interval can be found, for instance, in Gaustchi [8], Evans [5] and Krylov [10].

Gaussian quadratures are based on the choice of the nodes x_1, x_2, \dots, x_n as roots of an orthogonal polynomial O_n of degree n . Here we do not address the computation of these roots, we assume they are available.

The roots of an orthogonal polynomial are simple, real, and lie in the interval (a, b) (see Atkinson [1] or Gautschi [8]). Also, as it is easy to prove, any orthogonal polynomial O_j of degree j is orthogonal to any polynomial p of degree less than j .

The Theorem 2.1 applied to a n -point Gaussian rule enables us to recover well known results for the degree and error expression of this type of rules as shown in the next Proposition.

Proposition 3.1. *Let x_1, \dots, x_n be the roots of an orthogonal polynomial O_n of degree n . Consider $I(f) = \int_a^b w(x)f(x)dx$, where w is a weight function and $f \in C^{2n}([a, b])$.*

A Gaussian quadrature rule $G_n(f) = \sum_{i=1}^n a_i f(x_i)$ for approximating $I(f)$ has degree of precision $d = 2n - 1$. The respective error $E_n(f)$ is

$$E_n(f) = \frac{1}{\alpha^2} \frac{\|O_n\|^2}{(2n)!} f^{(2n)}(\xi), \quad (17)$$

where α is the coefficient of x^n in O_n , ξ some point in (a, b) , and the norm $\|O_n\|$ is the L^2 norm induced by the inner product (16).

Proof. Let B_0 and B be the bases, respectively for \mathbb{P}_{n-1} and \mathbb{P}_{2n} , defined by (3) and (4). By Theorem 2.1 it is sufficient to prove that $I(q_{2n}) \neq 0$ and $I(q_j) = 0$ for $n \leq j \leq 2n-1$. It is obvious that $I(q_{2n}) \neq 0$ since the polynomial q_n is the positive function $q_{2n} = (x-x_1)^2(x-x_2)^2 \cdots (x-x_n)^2$, and so $I(q_{2n}) = \int_a^b w(x)q_{2n}(x)dx > 0$. Hence, the degree of a n -point rule is at most $2n-1$.

Let us now prove that $I(q_{n+k}) = 0$, for all $0 \leq k \leq n-1$. For, consider the following basis of \mathbb{P}_{2n-1} :

$$\tilde{B} = \{O_0, O_1, \dots, O_n, O_n\varphi_1, O_n\varphi_2, \dots, O_n\varphi_{n-1}\},$$

where $\{O_0, O_1, \dots, O_n\}$ is an orthogonal polynomial basis of \mathbb{P}_n . Any polynomial q_{n+k} of degree $n+k$ (with $0 \leq k \leq n-1$) can be written as a (unique) linear combination of the elements of \tilde{B} , that is

$$q_{n+k}(x) = \sum_{i=0}^n \gamma_i O_i(x) + \sum_{j=1}^k \gamma_{n+j} O_n(x) \varphi_j(x). \quad (18)$$

For any integer $0 \leq k \leq n-1$, the integral $I(q_{n+k})$ is

$$\begin{aligned} I(q_{n+k}) &= \int_a^b w(x)q_{n+k}(x)dx = \langle q_{n+k}, \varphi_0 \rangle \\ &= \sum_{i=0}^n \gamma_i \langle O_i, \varphi_0 \rangle + \sum_{j=1}^k \gamma_{n+j} \langle O_n \varphi_j, \varphi_0 \rangle \\ &= \gamma_0 \langle O_0, \varphi_0 \rangle + \sum_{j=1}^k \gamma_{n+j} \langle O_n, \varphi_j \rangle = \gamma_0 \langle O_0, \varphi_0 \rangle, \end{aligned} \quad (19)$$

where the last two equalities follow from the fact that an orthogonal polynomial O_j of degree j is orthogonal to any polynomial of degree less than j .

Evaluating (18) at the nodes x_1, \dots, x_n , and taking into account these nodes are roots of both O_n and q_{n+k} , we obtain a homogeneous linear system $Bx = 0$, in the unknowns $\gamma_0, \gamma_1, \dots, \gamma_{n-1}$, such that the first column of B has all entries equal to 1. Thus, $\gamma_0 = 0$ and from (19) we get $I(q_{n+k}) = 0$.

It remains to show that the error expression has the form given in (17). As x_1, \dots, x_n are the roots of O_n , we have $O_n = \alpha(x-x_1) \cdots (x-x_n)$, where α is the coefficient of x^n in O_n . Then,

$$\|O_n(x)\|^2 = \langle O_n(x), O_n(x) \rangle = \alpha^2 \int_a^b w(x)O_n^2(x)dx = \alpha^2 \int_a^b w(x)q_{2n}(x)dx.$$

So, $I(q_{2n}) = \frac{1}{\alpha^2} \|O_n(x)\|^2$ and (17) follows from (7). \square

Example: Gauss-Legendre rule

The Legendre polynomials, usually denoted by P_n , are orthogonal with respect to the weight function $w(x) = 1$ in the integration interval $[-1, 1]$. The coefficient α and $\|P_n\|^2$ in the error expression (17) satisfy the following equalities (see, for instance Davis [4], p. 33):

$$\alpha = \frac{(2n)!}{2^n(n!)^2}, \quad \|P_n\|^2 = \frac{2}{2n+1}. \quad (20)$$

Thus, from (17), the error expression for the Gauss-Legendre rule is

$$E_{G_n}(f) = c_n f^{(2n)}(\xi) \quad \text{with } c_n = \frac{2^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3}, \quad \xi \in (-1, 1), \quad (21)$$

agreeing with the well known expression for the error of a n -point Gauss-Legendre rule (see, for instance, Atkinson [1], p. 276).

Computational remarks

The computational efficiency of the algorithm referred in Remark 2.1-2), either for the rules previously discussed or any other polynomial quadrature rule one may construct, deserve further studies. However, we have yet developed a *Mathematica* (Wolfram [16]) code for the referred algorithm which, for a given number n of nodes, produces a list $\{nodes, weights, c_n\}$, where c_n is the coefficient in the respective error expression $E_n(f)$. This code has been implemented for all the rules detailed in the previous section and the computed coefficients c_n agree with those in (13), (15) and (21). Whenever possible the elements of the mentioned list have been computed exactly, such as in the cases of Newton-Cotes, Adams-Bashford and Adams-Moulton rules. Our program has been also tested for the Gauss-Legendre rule for a wide range of nodes number. For this rule, when $2 \leq n \leq 5$, we obtained closed expressions for the respective pairs (W_n, c_n) , while for $6 \leq n \leq 256$ we have computed 100-digits of precision approximations for the weights. The computations were carried out on a small laptop. The control of the error in the computation of the weights has been monitored taking into account that the sum of the weights satisfy the equality $\sum_{i=1}^n a_i = 2$, and knowing that all the weights in W_n are positive. Our numerical results were compared with those available in some published tables: for $2 \leq n \leq 512$, Stroud and Secrest ([15], p. 99), [30S]; for $2 \leq n \leq 48$, Krylov ([10], p. 337), [20S]; for $2 \leq n \leq 128$, Evans ([5], p. 303), [30S]; for $2 \leq n \leq 16$, Kythe

and Schäferkötter ([11], p. 505), [16*S*] – the symbol kS means k significant digits in the corresponding table.

We consider our high precision *in situ* computation of nodes, weights, and error coefficients for the n -point Gauss-Legendre’s rule a tribute to the pioneering work of Lowan, Davids and Levenson [12] and [13], who managed to publish a 16-digits precision Gauss-Legendre table, for $2 \leq n \leq 16$, in the terrible years of WWII.

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